TeXsor3DG

An Explicit 3D Cartesian Discontinous Galerkin Spectral Element Compressible Navier-Stokes Solver

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Motivation



High order methods in aerodynamics
Higher accuracy with fewer degrees of freedom
Fewer elements needed
Nodal Discontinuous Galerkin finite elements
Cartesian Setting-Higher efficiency per degree of freedom

Governing Equations



Compressible Navier-Stokes equations

$$\frac{\partial U_m}{\partial t} + \frac{\partial F_{mi}}{\partial x_i} = 0$$

Conservative variables $U = \{\rho, \rho u, \rho v, \rho w, \rho E\}^T$

$$F = \left\{ \begin{array}{cccc} \rho u & \rho v & \rho w \\ \rho u^2 + P - \tau_{11} & \rho uv - \tau_{12} & \rho uw - \tau_{13} \\ \rho uv - \tau_{21} & \rho v^2 + P - \tau_{22} & \rho vw - \tau_{23} \\ \rho uw - \tau_{31} & \rho vw - \tau_{32} & \rho w^2 + P - \tau_{33} \\ \rho uH - \tau_{1j}u_j + q_1 & \rho vH - \tau_{2j}u_j + q_2 & \rho wH - \tau_{3j}u_j + q_3 \end{array} \right\}$$

$$\rho E = \frac{P}{\gamma - 1} + \frac{1}{2}\rho(u^2 + v^2 + w^2)$$

DG Formulation



Multiply by test function and integrate

$$\int_{\Omega} \Psi_r \left(\frac{\partial U_m}{\partial t} + \frac{\partial F_{mi}}{\partial x_i} \right) \mathrm{d}\Omega = \int_{\Omega} \Psi_r S_m \mathrm{d}\Omega$$

Integrate by parts

$$R_{mr} = \int_{\Omega} \left(\Psi_r \frac{\partial U_m}{\partial t} - \Psi_r S_m - \frac{\partial \Psi_r}{\partial x_i} F_{mi} \right) d\Omega + \int_{\Gamma} \Psi_r F_{mi} n_i d\Gamma = 0$$

Inviscid flux: Lax-Friedrichs and Roe

Viscous flux: symmetric interior penalty (SIP)

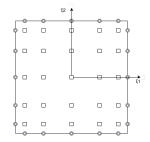
Tensor Basis Functions



Letting $\Psi_{ijk} = \phi_{\xi_i^1} \phi_{\xi_j^2} \phi_{\xi_k^3}$ for $i, j, k = 0, \dots, M$ and solution expansion coefficients a, written as:

$$U_{m}(\xi,t) = \sum_{k=0}^{M} \sum_{i=0}^{M} \sum_{j=0}^{M} a_{ijk}(t) \phi_{\xi_{i}^{1}} \phi_{\xi_{j}^{2}} \phi_{\xi_{k}^{3}}$$

Let $\phi_{\xi_i} = \mathcal{L}_i$, the 1-D Lagrange polynomial using the Gauss-Legendre quadrature points.





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 - solution coefficients are the solutions at the quadrature points – mass matrix is diagonal



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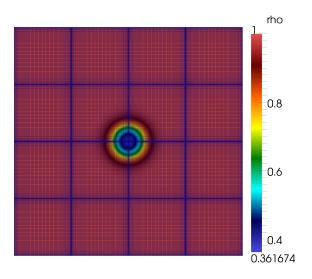
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- Polynomial degree of p=63
 - Restricted by CPU RAM on computing nodes (p=15)

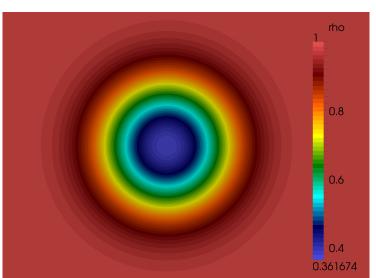
64th Order Solution





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Solver Capabilities Cont.



- Explicit time stepping through Method of Lines
 - Forward Euler
 - 4th-order explicit Runge-Kutta
 - Low-storage Runge-Kutta 3rd Order (near future)

¹Design of a Variational Multiscale Method for Turbulent Compressible Flows

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 - 4th-order explicit Runge-Kutta
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 - * explicit time step consistent with Laslo Diosady and Scott Murman¹

$$\delta t = min\left(\frac{S*h}{4(\|U\|+c)}, \frac{h^2}{\nu}\right)$$

$$h = \frac{min(dx, dy, dz)}{(p+1)^{2.5}}$$

$$S = \text{Number of Stages}$$

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• Parallel through MPI

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Validation Results: Ringleb Flow UNIVERSITY OF WVOMING



Problem Description²

Governing equations: 2D Euler equations with $\gamma = 1.4$

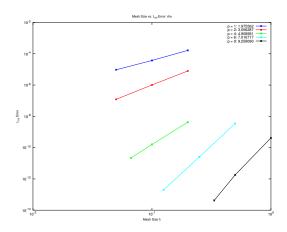


²http://www.as.dlr.de/hiocfd/case_c1.2.pdf

Validation Results: Ringleb-Rho UNIVERSITY OF WYOMING

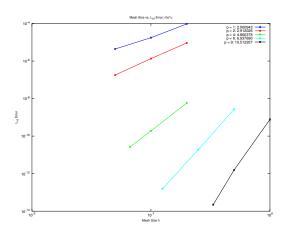


Р	1	2	4	6	9
Slope	1.975562	3.056287	4.90858	7.016717	9.259090



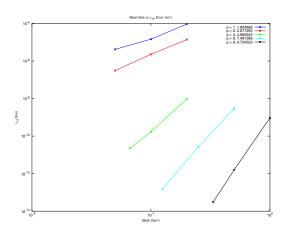
Validation Results: Ringleb-RhoU UNIVERSITY OF WYOMING

Р	1	2	4	6	9
Slope	2.000943	2.912026	4.860378	6.937690	10.51220



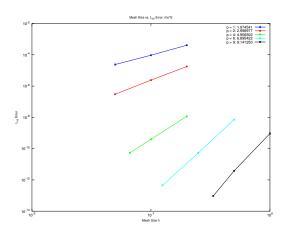
Validation Results: Ringleb-RhoV UNIVERSITY

	Р	1	2	4	6	9
Ī	Slope	1.804886	2.877250	4.990545	7.481386	9.754523



Validation Results: Ringleb-RhoE UNIVERSITY

Р	1	2	4	6	9
Slope	1.974541	2.998977	4.906502	6.895422	9.141250



Validation Results: Taylor Green Vortex WVOMING



Problem Description³

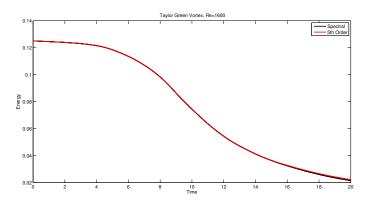
Domain:
$$[-\pi L, \pi L]^3$$
 $M_0 = 0.1$
 $Re = 1600$
 $Pr = 0.71$
 $u = V_0 \sin(x/L) \cos(y/L) \cos(z/L)$
 $v = -V_0 \cos(x/L) \sin(y/L) \cos(z/L)$
 $w = 0$
 $p = \rho_0 V_0^2 \left[\frac{1}{\gamma M_0^2} + \frac{1}{16} \left(\cos(2x) + \sin(2y) \right) \left(\cos(2z) + 2 \right) \right]$

Mesh: 64x64x64 p = 4 (5th order)

³http://www.as.dlr.de/hiocfd/case_c3.5.pdf

Validation Results: Taylor Green Vortex UNIVERSITY OF WYOMING

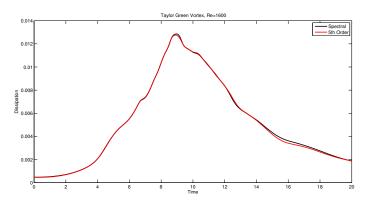




Energy

Validation Results: Taylor Green Vortex UNIVERSITY OF WYOMING

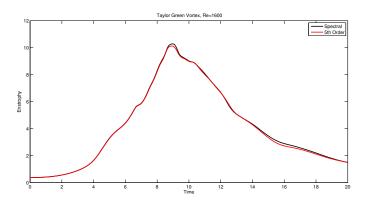




Dissipation

Validation Results: Taylor Green Vortex UNIVERSITY OF WYOMING





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Timing Results



All results are computed in serial on Intel Xeon E5-2670 processors with a clock speed of 2.6Ghz and 2GB per core memory.

• Mount Moran TAU benchmark = 7.2 sec

Mount Moran Specs:

- 93.92 Tflops cluster serving the University of Wyoming
- 218 nodes with 2, eight-core Intel Xeon E5-2670 Sandy Bridge processors on each node (3,488)

Timing Results: 3D Euler



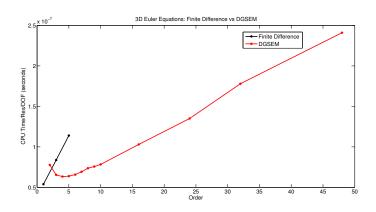
DOF= $(number of fields)(p+1)^3 NxNyNz$

Three-dimensional Euler Equations

Tillee-ullilensional Euler Equations						
Code	Order	DOF	Mesh Size	Time/Res/DOF		
Finite Difference	1	5,151,505	100 × 100 × 100	5.39e-8		
Finite Difference	3	5,151,505	$100\times100\times100$	8.37e-8		
Finite Difference	5	5,151,505	$100\times100\times100$	1.14e-7		
DGSEM	2	5,000,000	50×50×50	7.77e-8		
DGSEM	3	4,851,495	33x33x33	6.54e-8		
DGSEM	4	5,000,000	25×25×25	6.33e-8		
DGSEM	5	5,000,000	20×20×20	6.38e-8		
DGSEM	6	5,306,040	17×17×17	6.57e-8		
DGSEM	7	4,705,960	14×14×14	6.92e-8		
DGSEM	8	4,423,680	12×12×12	7.36e-8		
DGSEM	9	4,851,495	11×11×11	7.57e-8		
DGSEM	10	5,000,000	10×10×10	7.83e-8		
DGSEM	16	4,423,680	6×6×6	1.03e-7		
DGSEM	24	4,423,680	4×4×4	1.35e-7		
DGSEM	32	4,423,680	3x3x3	1.78e-7		
DGSEM	48	552,960	1×1×1	2.41e-7		

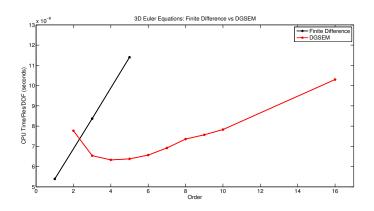
Timing Results: 3D Euler





Timing Results: 3D Euler





At 5th order, DGSEM is ∼twice as efficient!

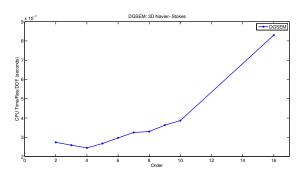
Timing Results: Cartesian 3D Navier-Stokes UNIVERSITY OF WYOMING

DOF=(number of fields) $(p+1)^3 NxNyNz$

Three-dimensional Compressible Navier-Stokes Equations

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Code	Order	DOF	Mesh Size	Time/Res/DOF	
DGSEM	2	5,000,000	50×50×50	2.74e-7	
DGSEM	3	4,851,495	33x33x33	2.59e-7	
DGSEM	4	5,000,000	25×25×25	2.45e-7	
DGSEM	5	5,000,000	20×20×20	2.68e-7	
DGSEM	6	5,306,040	17×17×17	2.97e-7	
DGSEM	7	4,705,960	14×14×14	3.25e-7	
DGSEM	8	4,423,680	12×12×12	3.30e-7	
DGSEM	9	4,851,495	11×11×11	3.63e-7	
DGSEM	10	5,000,000	10×10×10	3.87e-7	
DGSEM	16	4,423,680	6×6×6	8.30e-7	

Timing Results: Cartesian 3D Navier-Stokes UNIVERSITY



Laslo Diosady and Scott Murman $\approx 1.5e^{-7}$ (non-Cartesian) ⁴ F. Hindenlang, G. Gassner $\approx 4.0e^{-7}$ (non-Cartesian) ⁵

⁴Design of a Variational Multiscale Method for Turbulent Compressible Flows

⁵Explicit Discontinuous Galerkin methods for unsteady problems

Results: Parallel Scalability



- Strong Scalability
- Computed on Mount Moran and Yellowstone
- Taylor-Green Vortex

MPI Implementations:

- MPI Cartesian Topology
- MPI Derived Data Types
 - MPI_Type_Contiguous (x-y plane faces)
 - MPI_Type_Vector (x-z and y-z plane faces)

Yellowstone Strong Scalability Results



Following results are computed in parallel on Intel Xeon E5-2670 processors with a clock speed of 2.6Ghz and 2GB per core memory.

•Yellowstone TAU benchmark = 8.4 sec

Yellowstone Specs:

- 1.504-petaflops peak IBM iDataPlex cluster
- 2.6-GHz Intel Xeon E5-2670 (Sandy Bridge) processors with Advanced Vector Extensions (AVX), 8 flops per clock (72,576)
- 144.58 TB total system memory

Results: Strong Scalability P = 4



Mesh Size: Nx=128, Ny=128, NZ=128

DOF(total) = 1,310,720,000

DOF=(number of fields) $(p+1)^3 NxNyNz$

Yellowstone Strong Scaling Results: P = 4

# Procs	DOF per Proc	Efficiency
1024*	1,280,000	1.0000
2048	640,000	0.9801
4096	320,000	0.9327
8192	160,000	0.9037
16384	80,000	0.8358

^{*}Assumed Perfect

Results: Strong Scalability P = 7



Mesh Size: Nx=128, Ny=128, NZ=128

DOF(total) = 5,368,709,120

DOF=(number of fields) $(p+1)^3 Nx Ny Nz$

Yellowstone Strong Scaling Results: P = 7

# Procs	DOF per Proc	Efficiency
1024*	5,242,880	1.0000
2048	2,621,440	0.9923
4096	1,310,720	0.9793
8192	665,360	0.9580
16384	327,680	0.9210

^{*}Assumed Perfect

Results: Strong Scalability P = 9



Mesh Size: Nx=128, Ny=128, NZ=128

DOF(total) = 10,485,760,000

DOF=(number of fields) $(p+1)^3 NxNyNz$

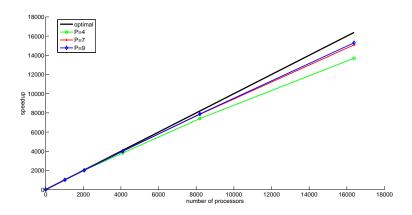
Yellowstone Strong Scaling Results: P = 9

# Procs	DOF per Proc	Efficiency
1024*	10,240,000	1.0000
2048	5,120,000	0.9877
4096	2,560,000	0.9768
8192	1,280,000	0.9633
16384	640,000	0.9340

^{*}Assumed Perfect

Results: Parallel Scalability





Future Work: Short Term Goals UNIVERSITY OF WYOMING



• Adaptive 3D Discontinuous Galerkin Navier-Stokes Solver

Future Work: Short Term Goals WVOMING



- Adaptive 3D Discontinuous Galerkin Navier-Stokes Solver
 - Tamrex3DG = TeXsor3DG + SAMRAL
 - analogous version of SAMARC
 - different solution orders on different blocks

Future Work: Short Term Goals WVOMING

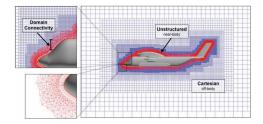


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- 3D Navier-Stokes Dual Mesh/Dual Flow Solver

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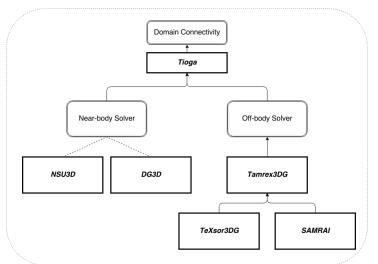
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 - analogous version of HELIOS



Future Work: Short Term Goals cont. UNIVERSITY OF WYOMING



3D Navier-Stokes Dual Mesh/Dual Flow Solver







- Use Tamrex3DG in HELIOS?
- Dynamic LES Model
 - possible dealiasing required



- Dynamic LES Model
 - possible dealiasing required
- Particle Tracking
 - implement scalar equation



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 - possible dealiasing required
- Particle Tracking
 - implement scalar equation
- Newton Implicit Solver
- Discrete Adjoint for design optimization and driver for AMR
- GPGPU version of TeXsor3DG

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- University of Wyoming Advanced Research Computing Center
- NASA Ames







